Introduction to the Theory of Spin Glasses

Chandan Dasgupta
Department of Physics
Indian Institute of Science
cdgupta@physics.iisc.ernet.in

School on Glass Formers and Glasses

JNCASR, Bangalore, January 2010

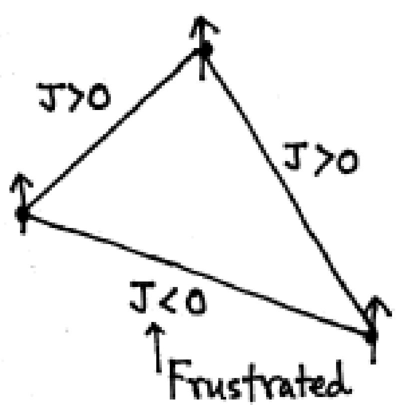
What are Spin Glasses?

Magnetic systems with **quenched disorder**.
Competition between ferromagnetic and antiferromagnetic Interactions.

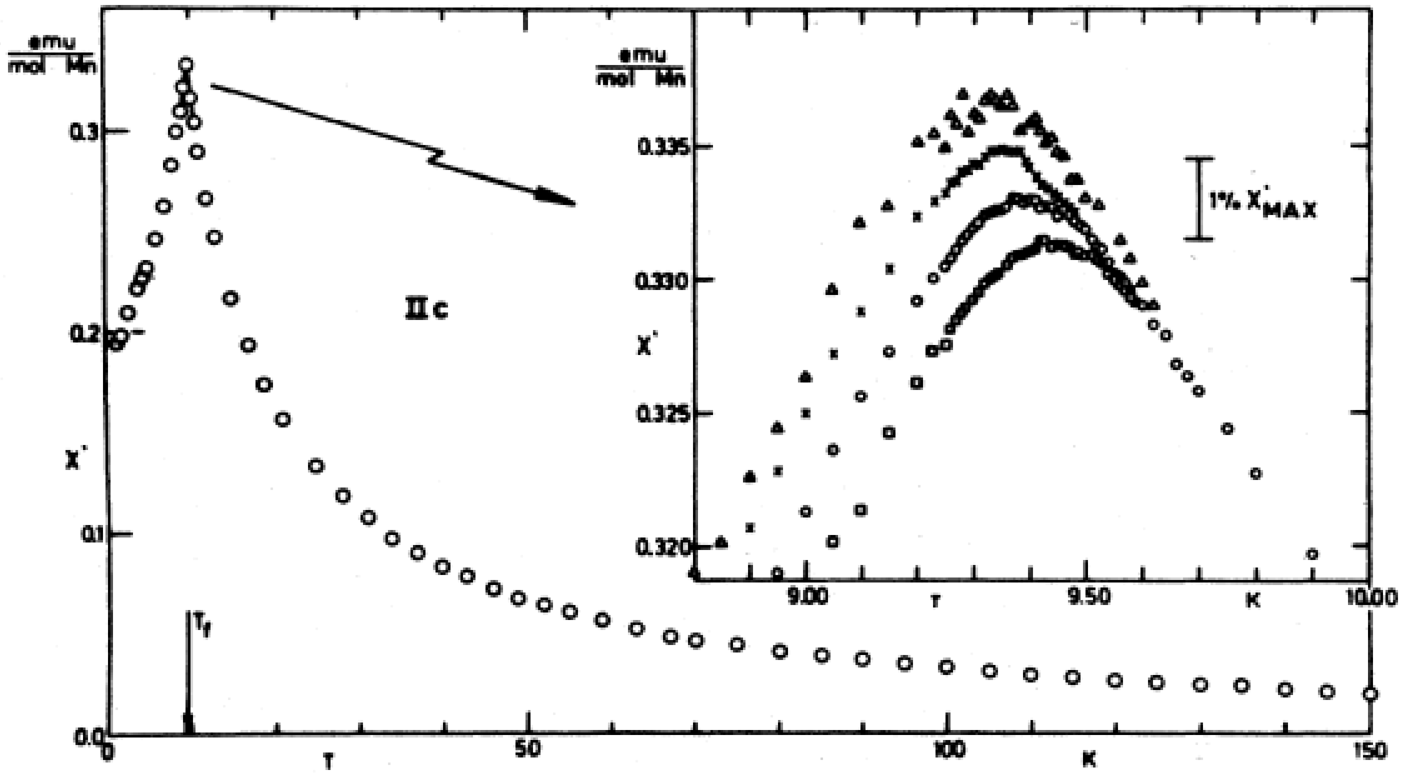
Example: CuMn, AuFe, …

RKKY Interaction:

$$J(R) = J_0 \frac{\cos(2k_F R + \phi_0)}{(k_F R)^3}$$



FRUSTRATION



Susceptibility of CuMn as a function of temperature

Figures from K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801 (1986).

Edwards-Anderson Model

S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

Ising spins, $\sigma_i = \pm 1$.

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j, \qquad J_{ij}\text{'s are random.}$$

$$P(\{J_{ij}\}) = \prod_{\langle ij \rangle} P(J_{ij})$$

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J^2}} e^{-J_{ij}^2/2J^2}$$

$$\text{or } P(J_{ij}) = \frac{1}{2}\delta(J_{ij} - J) + \frac{1}{2}\delta(J_{ij} + J)$$

So that $[J_{ij}]_{av} = 0$, $[J_{ij}^2]_{av} = J^2$

No ferromagnetic or antiferromagnetic phase is possible

Spin Glass Phase

High temperature : $\langle \sigma_i \rangle = 0$

Paramagnetic Phase.

Low temperature : $\langle \sigma_i \rangle \neq 0$

$$M = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle = 0$$

Spin glass phase

$$q = \frac{1}{N} \sum_i \langle \sigma_i \rangle^2 \neq 0$$

Edwards - Anderson order parameter.

$$C(t) = \frac{1}{N} \sum_i \left\langle \sigma_i(t_0)\, \sigma_i(t_0+t) \right\rangle$$

$$\lim_{t \to \infty} C(t) = \frac{1}{N} \sum_i \langle \sigma_i \rangle^2 = q \neq 0$$

in the spin glass phase

Spin glass transition :
"Freezing" of the spins
in random orientations

The Replica Method

Configuration averaged free energy

$$F = Nf = -T\left[\ln Z(\{J_{ij}\})\right]_{av}$$

$$= -T\int \prod dJ_{ij}\, P(\{J_{ij}\}) \ln Z(\{J_{ij}\})$$

Identity $\quad \ln x = \lim_{n\to 0} \frac{x^n - 1}{n}$

$$\Rightarrow \ln Z = \lim_{n\to 0} \frac{Z^n - 1}{n}$$

$$\left[\ln Z(\{J_{ij}\})\right]_{av} = \lim_{n\to 0} \frac{1}{n}\left[\left[Z^n(\{J_{ij}\})\right]_{av} - 1\right]$$

$$\left[Z^n(\{J_{ij}\})\right]_{av} = \mathrm{Tr}_{\{\sigma_i^\alpha\}} \left[e^{-\beta \sum_{\alpha=1}^{n} \mathcal{H}(\{J_{ij}\},\{\sigma_i^\alpha\})} \right]_{av}$$

$$= \mathrm{Tr}_{\{\sigma_i^\alpha\}} \, e^{-\beta \mathcal{H}_{eff}(\{\sigma_i^\alpha\})}$$

$$\mathcal{H}_{eff} = -T \ln \left[\int \prod dJ_{ij} \, P(\{J_{ij}\}) \, e^{-\beta \sum_{\alpha=1}^{n} \mathcal{H}(\{J_{ij}\},\{\sigma_i^\alpha\})} \right]$$

does not have any randomness.

Edwards-Anderson (Spin Glass) Order Parameter

$$q = \left[\langle \sigma_i \rangle^2\right]_{av} = \langle \sigma_i^\alpha \sigma_i^\beta \rangle_{\mathcal{H}_{eff}}, \quad \alpha \neq \beta.$$

The spin glass transition is from the paramagnetic state with q=0 to a spin glass state with nonzero q as the temperature is decreased.

The Sherrington-Kirkpatrick Model

D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1972 (1975).

Infinite-range (mean field) model of Ising spin glass

$$\mathcal{H} = -\frac{1}{2}\sum_{i \neq j} J_{ij}\sigma_i\sigma_j = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j$$

$$P(J_{ij}) = \frac{1}{J}\left(\frac{N}{2\pi}\right)^{1/2} \exp\left[-NJ_{ij}^2/2J^2\right]$$

$$[J_{ij}]_{av} = 0, \qquad [J_{ij}^2]_{av} = J^2/N.$$

$$[Z^n]_{av} = \mathrm{Tr}_{\{\sigma_i^\alpha\}} \exp\left[\frac{1}{N}\sum_{\langle ij \rangle}\frac{1}{2}\beta^2 J^2 \sum_{\alpha,\beta}\sigma_i^\alpha\sigma_i^\beta\sigma_j^\alpha\sigma_j^\beta\right]$$

Hubbard - Stratanovitch identity:

$$e^{\lambda a^2/2} = \left(\frac{\lambda}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty} dx\, e^{-\frac{\lambda x^2}{2} + \lambda a x}$$

S-K Model (contd.)

$$\Rightarrow [Z^n]_{av} = e^{\frac{1}{4}\beta^2 J^2 nN} \int_{-\infty}^{\infty} \prod_{\alpha<\beta} \left(\frac{N}{2\pi}\right)^{1/2} \beta J \, dq_{\alpha\beta}$$

$$\times \exp\left[-\frac{N\beta^2 J^2}{2} \sum_{\alpha<\beta} q_{\alpha\beta}^2 + N \ln \mathrm{Tr}_{\{\sigma^\alpha\}} e^{L(\{q_{\alpha\beta}\})}\right]$$

where

$$L(\{q_{\alpha\beta}\}) \equiv \beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} \sigma^\alpha \sigma^\beta$$

$$\Rightarrow -\beta f = \lim_{n\to 0} \left[\frac{\beta^2 J^2}{4}\left(1 - \frac{1}{n}\sum_{\alpha,\beta} q_{\alpha\beta}^2\right) + \frac{1}{n} \ln \mathrm{Tr}\, e^{L}\right]$$

where $q_{\alpha\beta}$ is to be determined by

$$\frac{\partial f}{\partial q_{\alpha\beta}} = 0.$$

S-K Model (contd.)

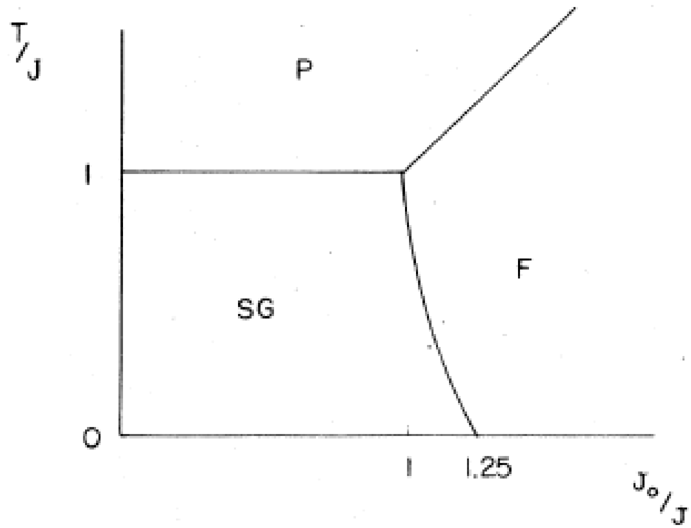
Replica symmetry: $q_{\alpha\beta} = q$ for all $\alpha \neq \beta$.

Self-consistency:

$$q = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz\, e^{-z^2/2} \tanh^2\left(\beta J \sqrt{q}\, z\right)$$

$q \neq 0$ for $T < T_c = J \Leftarrow$ spin glass transition

Phase diagram



Replica Symmetry Breaking

The replica symmetric solution has unphysical properties for T < J.

Instability of the replica symmetric solution

$$-\beta f = \lim_{n\to 0}\left[\frac{\beta^2 J^2}{4}\left(1-\frac{1}{n}\sum_{\alpha\beta} q_{\alpha\beta}^2\right)+\frac{1}{n}\ln \mathrm{Tr}\, e^{L}\right]$$

$$q_{\alpha\beta} = q_0 + \delta q_{\alpha\beta}$$

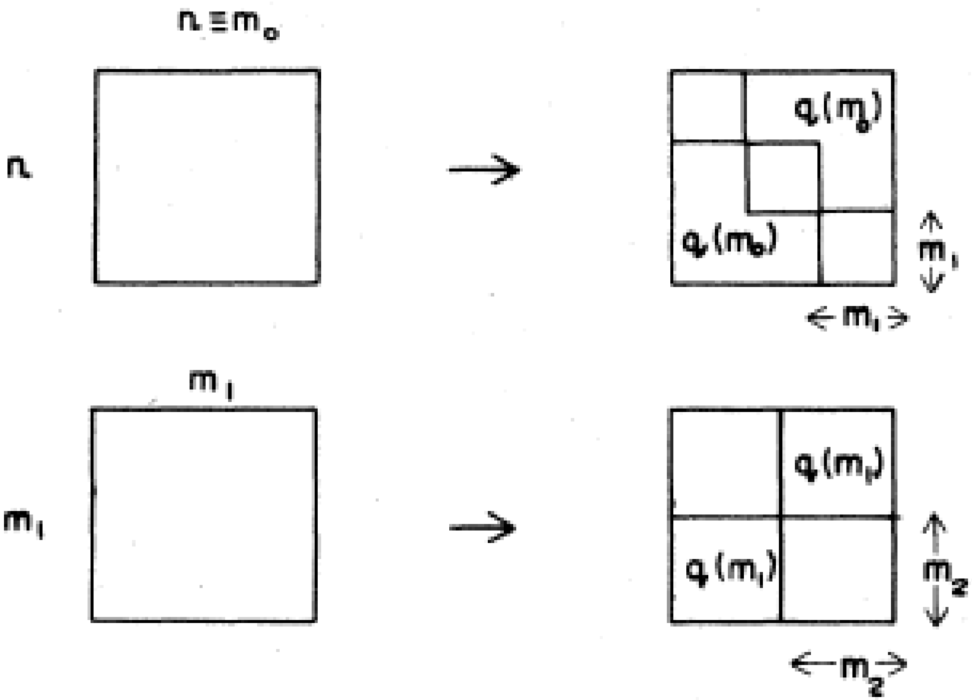
$$\beta f = \beta f(q_0) + \lim_{n\to 0}\frac{1}{2n}\sum_{\substack{\alpha<\beta\\ \gamma<\delta}} R^{\alpha\beta,\gamma\delta}\,\delta q_{\alpha\beta}\,\delta q_{\gamma\delta} + \cdots$$

All eigenvalues of R must be ≥ 0 for stability and physically meaningful behavior.

This condition is not satisfied for $T<J$.

The Parisi Solution

G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979)



Repeat this procedure K times: K-step Replica Symmetry Breaking (RSB)

$m_1, m_2, \cdots, m_K$; $0 \le m_i \le 1$

$q(m_1), q(m_2), \cdots, q(m_K)$

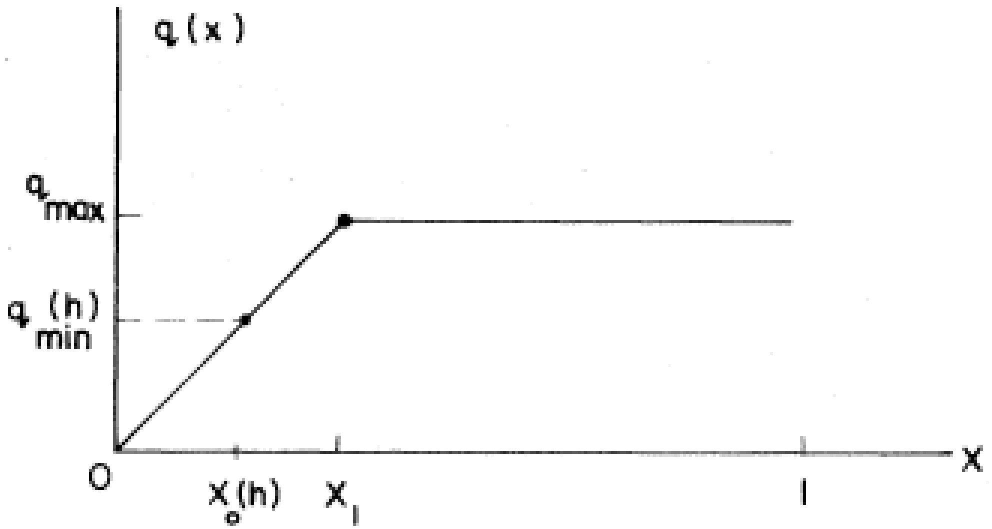
The Parisi Solution

$K \to \infty$: $m_i \to x$, $0 \leq x \leq 1$.

$q(m_i) \longrightarrow q(x)$: Order parameter <u>function</u> of Parisi

Spin glass order parameter

$$q = [\langle \sigma_i \rangle^2]_{av} = \int_0^1 q(x)\, dx$$



q(x) at a temperature slightly below the critical temperature

The Thouless-Anderson-Palmer Equations

Philosoph. Mag. 35, 593 (1977)

Free energy of the S-K model for a given set of $\{J_{ij}\}$.

$$F = -\frac{1}{2}\sum_{i\neq j} J_{ij}\, m_i m_j + \frac{T}{2}\sum_i \left[(1+m_i)\ln\left(\frac{1+m_i}{2}\right) + (1-m_i)\ln\left(\frac{1-m_i}{2}\right)\right] - \frac{1}{4T}\sum_{i\neq j}(1-m_i^2)(1-m_j^2)\,J_{ij}^2$$

Onsager reaction term

$$m_i = \langle \sigma_i \rangle$$

$$\frac{\partial F}{\partial m_i} = 0 \Rightarrow m_i = \tanh\left[\beta \sum_j J_{ij}\, m_j - \beta \sum_j J_{ij}^2 (1-m_j^2)\, m_i\right]$$

TAP Equations

Eigenvalues of $\frac{\partial^2 F}{\partial m_i \partial m_j}$ must be ≥ 0.

Only one solution, $m_i = 0$ for all i, for $T > J$.

Exponentially large number of solutions for $T < J$.

Number of minima with the lowest free energy per spin is not exponential in N.

Free energy barriers between different minima diverge in the thermodynamic limit.

Complex Free Energy Landscape

Physical interpretation of RSB

Large number of "valleys" ["pure states", "ergodic components"] at temperatures lower than the critical temperature.

$P^{(\alpha)}$: Probability of the system being in valley α.

$$\langle \sigma_i \rangle = \sum_{\alpha} P^{(\alpha)} m_i^{(\alpha)}$$

$$\frac{1}{N} \sum_i \langle \sigma_i \rangle^2 = \frac{1}{N} \sum_i \sum_{\alpha,\beta} m_i^{(\alpha)} m_i^{(\beta)} P^{(\alpha)} P^{(\beta)}$$

Define overlap $q^{\alpha\beta} = \frac{1}{N} \sum_i m_i^{(\alpha)} m_i^{(\beta)}$

and $P(q) = \sum_{\alpha\beta} P^{(\alpha)} P^{(\beta)} \delta(q - q^{\alpha\beta})$

$$\Rightarrow \frac{1}{N} \sum_i \langle \sigma_i \rangle^2 = \int q \, P(q) \, dq$$

Compare with the replica theory result,

$$\frac{1}{N}\sum_i \langle \sigma_i \rangle^2 = \int q(x)\,dx = \int q \frac{dx}{dq}\,dq$$

$$\boxed{P(q) = \frac{dx}{dq}}$$

Parisi function q(x) describes the distribution of overlaps between different free-energy minima.

$$q_{EA} \equiv \frac{1}{N}\sum_{\alpha} P^{(\alpha)}\left[m_i^{(\alpha)}\right]^2 = q(x=1)$$

Spin Glass Models Relevant to Structural Glasses

1. Potts glass

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \left[s\,\delta_{\sigma_i \sigma_j} - 1 \right]$$

Each σ_i can take s values

2. Ising spin glass with p-spin interactions

$$\mathcal{H} = -\sum_{\langle i_1, \dots, i_p \rangle} J_{i_1 \dots i_p} \sigma_{i_1} \sigma_{i_2} \cdots \sigma_{i_p}$$

RANDOM FIRST ORDER TRANSITION

Spin-glass-like Theories

[Kirkpatrick, Thirumalai, Wolynes, Parisi, Mézard, Monasson, Franz,...]

Infinite-range Potts glasses and Ising spin glasses with multi-spin interactions

Dynamical Transition to non-ergodic behaviour at $T = T_d$

Dynamics for $T \to T_d^+ \approx$ Ideal MCT

Thermodynamics for $T < T_d$ governed by an exponentially large number of local minima of the free energy.

For $T < T_d$:

$$F(T) = -T \ln \sum_k \exp(-F_k/T) = \langle F_k \rangle - T S_c(T)$$

$S_c(T)$ is the extensive "configurational entropy" or "complexity" of the free-energy minima

$S_c(T)/N \to 0$ as $T \to T_s^+$ ($T_s < T_d$)
Thermodynamic transition at T_s, described by one-step replica symmetry breaking

<u>Connection with the glass transition:</u>
Dynamical transition at $T_d \approx$ Crossover at T_c
Static transition at $T_s \approx$ Thermodynamic transition at $T_0 = T_K$

Questions:

- No quenched disorder in supercooled liquids
  Self-generation of "quenched" disorder in models with frustration

- Need to carry out calculations for models of interacting particles
  Liquid-state methods and density functional theory
  CD , M. Mezard

- Need to go beyond mean-field theory by including effects of fluctuations neglected in mean-field treatments ??

- Dynamics of supercooled liquids for temperatures $T_c > T > T_0$??
  Kirkpatrick, Thirumalai and Wolynes (1989): VFT behaviour from "mosaic structure" formed via "entropic" nucleation

$$\boxed{\text{Random First Order Transition (RFOT) Theory of the Dynamics of Supercooled Liquids}}$$